Boundary of the Set of Separable States

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Abstract

The set of all separable quantum states is compact and convex. We focus on the two-qubit quanum system and study the boundary of the set. Then we give the criterion to determine whether a separable state is on the boundary. Some straightforward geometrical interpretations for entanglement are based on the concept and presented subsequently.

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I. INTRODUCTION

Entanglement and nonlocality are some of the most emblematic concepts embodied in quantum mechanics [1,2]. Recent developments in quantum computation [3,4] and quantum information (e.g. [5–7]) evoke interest in the properties of quantum entanglement.

Now we have known that a state of a composite quantum system is called entangled (or inseparable) if it cannot be represented as a convex combination of tensor products of its subsystem states [4,8]. In the case of pure states, one has obtained a complete understanding, that is, a pure state is entangled if and only if it violates Bell's inequality [9–11]. But the case for mixed states is much more complicated (e.g. [12,13]). Besides the above definition of entangled state, another qualitative criterion proposed by Peres [14] is more practicable to determine whether a given state is inseparable, although it is sufficient and necessary only for sone simple quantum system, such as 2×2 and 2×3 systems. On the other hand, one is more interested in the quantitative measure of entangled states. Various entanglement measure has been proposed. For example, for two-party system, there are following kinds of measure: the entanglement of formation [4], the relative entropy of entanglement [15,16], and the robustness of entanglement [17], *etc.*

Consider the relative entropy associated with entangled state ρ_e of two-qubit system. In order to obtain the relative entropy of entanglement of ρ_e, the crucial point is to find a separable state ρ_s such that minimizes the relative entropy $S\left(\rho_e \parallel \rho_s\right)$ defined as

$$S\left(\rho_e \parallel \rho_s\right) = tr\left\{\rho_e \ln \frac{\rho_e}{\rho_s}\right\}. \tag{1}$$

In general case, to find ρ_s is a laborious work.

Then recall the robustness of entanglement. It is said that given an entangled state ρ_e and a separable state ρ_s there always exists a minimal real $s \geqslant 0$ for which

$$\rho\left(s\right) = \frac{1}{1+s}\left(\rho_e + s\rho_s\right) \tag{2}$$

is separable. Such minimal s, denoted by $R\left(\rho_e \parallel \rho_s\right)$, is called robustness of ρ_e relative to ρ_s. Then the entanglement embodied in ρ_e can be measured by the absolute robustness of ρ_e, which is obtained by means of finding a separable state ρ_s' such that $R\left(\rho_e \parallel \rho_s'\right)$ is minimal. We can see that both in relative entropy and in robustness, finding a specific separable state is of essence.

Additionally, let's consider another useful tool to study entanglement, *i.e.*, Lewenstein-Sanpera (L-S) decomposition [18]. Lewenstein *et.al.* have shown that any state of two-qubit system can be decomposed as

$$\rho = \lambda\rho_s + \left(1 - \lambda\right)P_e, \quad \lambda \in \left[0.1\right], \tag{3}$$

where ρ_s is a separable state, and P_e denotes a single pure entangled projector ($P_e = |\Psi_e\rangle\langle\Psi_e|$), that is, P_e represents a pure entangled state. It is known that there are many different L-S decomposition with varying values of λ and various P_e's. Among them is the unique optimal decomposition, the one with the largest λ value in Eq. (3),

$$\rho = S\rho_s^{(opt)} + (1 - S)P_e^{(opt)}, \tag{4}$$

where

$$S = \max\left\{\lambda\right\}$$

is the degree of separability possessed by ρ. In other words, the entanglement possessed by ρ can be represented as $(1 - S)E\left(\Psi_e\right)$, where $E\left(\Psi_e\right)$ is the entanglement of its pure state

expressed in terms of the von Neumann entropy of the reduced density matrix of either of its subsystems:

$$E\left(\Psi_e\right) = -tr\left(\rho_A \log \rho_A\right) = -tr\left(\rho_B \log \rho_B\right). \tag{5}$$

Here again, in the sense of maximizing or minimizing some quality, a specific separable state $\rho_s^{(opt)}$ appears.

From the above consideration, we show that there are some specific separable states playing an important role in determining the entanglement measure. Then it is meaningful to determine the properties of these separable states. A fact provokes our attention. That is, at least for two-qubit system the set of separable states, denoted by $\mathcal{S}$, is compact and convex [19]. Then boundary of $\mathcal{S}$ does exist. We argue in this paper that these special separable states mentioned above are on the boundary of $\mathcal{S}$. In the following, we give the criterion to determine whether a separable state is on the boundary. Taking this into account, we present more clear interpretations on some concepts concerning quantum entanglement.

II. BOUNDARY OF $\mathcal{S}$

In this paper, we focus on the two-qubit quantum system. The states can be represented in the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$. So we also call it 2×2 quantum system. We know that all 4×4 Hermitian matrices span a 16-dimensional real Hilbert space, denoted by $\mathcal{H}$. All density matrices of states forms a subset of $\mathcal{H}$. We choose Hilber-Schimdt metric, that is, for $A \in \mathcal{H}$, the norm is defined as $\|A\| = [tr\left(A^+A\right)]^{\frac{1}{2}} = [tr\left(A^2\right)]^{\frac{1}{2}}$, and for $A, B \in \mathcal{H}$, the distance of A and B is

$$\|A - B\| = \left[tr\left(A - B\right)^2\right]^{\frac{1}{2}}. \tag{6}$$

For two-qubit system,a given state ρ is separable, i.e. $\rho \in \mathcal{S}$, if and only if the partial transposition of ρ ,denoted by ρ^{T_b} or ρ^{T_a} ($\rho^{T_b} = (\rho^{T_a})^*$), is also positive [14,19], or equivalently, the partial time-reversal of ρ, denoted by $\widetilde{\rho}$, is positive. Consider an arbitrary separable state $\rho_s \in \mathcal{S}$. Mixing it with the maximal separable state $\rho_0 = \frac{1}{4}I_{4\times4}$, we have

$$\rho_\varepsilon = (1 - \varepsilon)\, \rho_0 + \varepsilon \rho_s, \quad \varepsilon \in [0, 1]. \tag{7}$$

Obviously, $\rho_\varepsilon \in \mathcal{S}$ for each ε. In the geometrical view, ρ_ε is on the line segment connecting ρ_s and ρ_0, Then consider another form of mixture of ρ_s and ρ_0,

$$\rho_{\varepsilon'} = (1 - \varepsilon')\, \rho_0 + \varepsilon' \rho_s \qquad \varepsilon' > 1. \tag{8}$$

At this time, $\rho_{\varepsilon'}$ is on the extension line from ρ_0 to ρ_s. From the theorems in [20], we know that $\rho_{\varepsilon'}$ can be in the interior of $\mathcal{S}$, on the boundary of $\mathcal{S}$, or outside of $\mathcal{S}$. That depends on the values of ε'. So for sufficiently large $\varepsilon' > 1$, $\rho_{\varepsilon'}$ may be outside of $\mathcal{S}$.

Let us now obtain our main result, which refer to the boundary of $\mathcal{S}$.

THEOREM For a given separable state $\rho_b \in \mathcal{S}$, if and only if either of the following conditions is satisfied, ρ_b is on the boundary of $\mathcal{S}$,

(i) there exists at least one vanishing eigenvalue for ρ_b;

(ii) there exists at least one vanishing eigenvalues for $\widetilde{\rho}_b$.

or in the other words, the rank of ρ_b or $\widetilde{\rho}_b$ is no larger than 3.

Proof Note that $\mathcal{S} \in \mathcal{H}$ and $\mathcal{S}$ is compact and convex and that ρ_0 is in the interior of $\mathcal{S}$. If ρ_b is on the boundary of $\mathcal{S}$, let us consider the mixture with form of Eq.(8), that is,

$$\rho_\delta = (1 - \delta)\rho_0 + \delta\rho_b, \quad \delta > 1. \tag{9}$$

From [20], we know that such ρ_δ does not belong to $\mathcal{S}$. Therefore, for a given $\delta > 1$, there are two possibilities for ρ_δ . That is, either ρ_δ is positive and thus represents an entangled state, or ρ_δ is non-positive and does not represent any physical state. In the former case, any point on the line segment from ρ_0 to ρ_δ represents a real physical state, and particularly, all the points (except ρ_b) on the line segment from ρ_b to ρ_δ are entangled states. Let $\delta \to 1$, then $\rho_\delta \to \rho_b$. Correspondingly $\widetilde{\rho}_\delta \to \widetilde{\rho}_b$. Under this condition, the distance between ρ_b and ρ_δ can be arbitrarily small. Note that both ρ_b and $\widetilde{\rho}_b$ are clearly positive and that ρ_δ is also positive. But $\widetilde{\rho}_\delta$ is non-positive. So by connectivity of the space and continuity of δ we conclude that $\widetilde{\rho}_b$ must have vanishing eigenvalue. For the other case in which ρ_δ is

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non-positive and does not represent real state, similar analysis shows that ρ_b has at least one vanishing eigenvalue.

To prove the reverse. We first consider a separable state ρ_s the eigenvalues of which can be denoted by $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 = 0$, that is, ρ_s has at least one vanishing eigenvalue. We assume that ρ_s is in the interior of $\mathcal{S}$. Due to the compactness and convexity of $\mathcal{S}$ and with the help of [20], we know that there always exists a $\varepsilon' > 1$ such that the mixture $\rho_{\varepsilon'}$ in the form $\rho_{\varepsilon'} = (1 - \varepsilon')\rho_0 + \varepsilon'\rho_b$ $(\varepsilon' > 1)$ is also in the interior of $\mathcal{S}$. The eigenvalues of $\rho_{\varepsilon'}$, denoted by λ_i', can be easily calculated, that is,

$$\lambda_i' = \varepsilon'\lambda_i + \frac{1 - \varepsilon'}{4}, \quad (i = 1, \cdots, 4). \tag{10}$$

Obviously, for $\lambda_4 = 0$, we have $\lambda_4' = \frac{1-\varepsilon'}{4} < 0$. Then ρ_ε' is non-positive and can not belong to $\mathcal{S}$. This result contradicts with the assumption made above. Hence ρ_s can not be in the interior and can only be on the boundary of $\mathcal{S}$, i.e. $\rho_s = \rho_b$. On the other hand, let's consider a separable state ρ_s such that $\widetilde{\rho}_s$ has one vanishing eigenvalue, $i.e.$ $\widetilde{\lambda}_1 \geq \widetilde{\lambda}_2 \geq \widetilde{\lambda}_3 > \widetilde{\lambda}_4 = 0$. Also assume that ρ_s is in the interior of $\mathcal{S}$. Then $\rho_{\varepsilon'}$ is the interior point of $\mathcal{S}$ for some $\varepsilon' > 1$. So $\widetilde{\rho}_{\varepsilon'}$ is necessarily positive. Denote the eigenvalues of $\widetilde{\rho}_{\varepsilon'}$ by $\widetilde{\lambda}_i', i = 1, \cdots 4$. Similar analysis will demonstrate that one of the eigenvalues of $\widetilde{\rho}_{\varepsilon'}$, which is actually $\widetilde{\lambda}_4$, is negative. It is contrary to the assumption. So $\rho_s = \rho_b$.

III. DISCUSSION

Having obtained the description of the boundary of $\mathcal{S}$, we now return to think about some concepts of quantum entanglement.

A. Relative Entropy of Entanglement

In [15,16], Vedrel $et.al.$ propose the concept of relative entropy of entanglement and give the numberical results for some examples of two-qubit entangled states. For instance, given entangled state ρ_e as

$$\rho_e = \lambda \left| \Phi^+ \right\rangle \left\langle \Phi^+ \right| + (1 - \lambda) \left| 01 \right\rangle \left\langle 01 \right|, \quad \lambda \in (0, 1), \tag{11}$$

where $\left| \Phi^+ \right\rangle = \frac{1}{\sqrt{2}} (\left| 00 \right\rangle + \left| 11 \right\rangle)$. The separable state which minimize the relative entropy $S(\rho_e \parallel \rho_s)$ (cf. Eq.(1)) is said to be

$$\rho_s = \frac{\lambda}{2} \left(1 - \frac{\lambda}{2} \right) \left| 00 \right\rangle \left\langle 00 \right| + \frac{\lambda}{2} \left(1 - \frac{\lambda}{2} \right) (\left| 00 \right\rangle \left\langle 11 \right| + H.C.)$$
$$+ \left(1 - \frac{\lambda}{2} \right)^2 \left| 01 \right\rangle \left\langle 01 \right| + \frac{\lambda^2}{4} \left| 10 \right\rangle \left\langle 10 \right| + \frac{\lambda}{2} \left(1 - \frac{\lambda}{2} \right) \left| 11 \right\rangle \left\langle 11 \right| \tag{12}$$

Straightforward computation shows that ρ_s has a vanishing eigenvalue. Then ρ_s is on the boundary of $\mathcal{S}$. This result also holds in the other examples mentioned in [15,16]. So we can say, at least for these specific cases, the relative entropy of entanglement can be achieved on the boundary of the set of separable states. It is possible to generalize this result.

B. Robustness of Entanglement

Recall that the robustness of entanglement proposed by Vidal *et al.* [17]. The geometrical interpretation has been obtained in [21], in which the boundary of $\mathcal{S}$ is not yet explicitly defined. The discussion in this Letter can be supplementary to [21]. We can say that for a given entangled state ρ_e of two-qubit system, if s in Eq.(2) is minimal among all separable states ρ_s, *i.e.* s is the absolute robustness of ρ_e, then ρ_s and $\rho(s)$ in Eq.(2) are necessarily on the boundary of $\mathcal{S}$.

C. Lewenstein-Sanpera Decomposition

Now let us give our interpretation for L-S decomposition. Recall the form of L-S decomposition represented by Eq.(3). Using Hilbert-Schmidt metric defined by Eq.(6), we can express the λ in Eq. (3) as

$$\lambda = \frac{\|\rho - P_e\|}{\|\rho_s - P_e\|}. \tag{13}$$

As shown in Fig.1, λ can be regarded as the ratio of the length of line segment AB to that of AC. With P_e (point A in Fig. 1) and ρ (point B) fixed, λ reaches the maximal when ρ_s

is on the boundary of $\mathcal{S}$, *i.e.*, the length of AC is minimal. In the geometrical view, this result is straightforward. So we can always rewrite Eq. (5) as

$$\rho = \eta \rho_b + (1 - \eta)\, P_e, \quad \lambda \in [0, 1], \tag{14}$$

where ρ_b is on the boundary and η is the maximal λ associated with P_e. Obviously,for Eq.(4) $\rho_s^{(opt)}$ is on the boundary of $\mathcal{S}$ and can be written as $\rho_b^{(opt)}$ while S can be expressed as $S = \max\{\eta\}$.

In [22], Englert *et al.* have erred to what is involved in L-S decomposition, that is, if $\rho = S\rho_b^{(opt)} + (1-S)P_e^{(opt)}$ is the optimal decomposition, then (a) the state $(1+\varepsilon)^{-1}(\rho_b^{(opt)} + \varepsilon P_e^{(opt)})$ is non-separable for $\varepsilon > 0$; and (b) the state $\rho_b^{(opt)} + (\frac{1}{S} - 1)(P_e^{(opt)} - P_e')$ is either non-positive or non-separable for each $P_e' \neq P_e^{(opt)}$. It is said in [16] that their verification is rather complicated even in seemingly simple cases. But in our view, it is easy to understand. Now we give our explanation as follows.

For conclusion (a), since the optimal decomposition of ρ has been obtained, $\rho_b^{(opt)}$ is necessarily on the boundary of $\mathcal{S}$. Thus the convexity of $\mathcal{S}$ guarantees that all points on the line segment AD (cf Fig. 1) can not belong to $\mathcal{S}$ and without choice represent entangled states. These states are expressed as the convex sum of $P_e^{(opt)}$ and $\rho_b^{(opt)}$, i.e., $(1+\varepsilon)^{-1}(\rho_b^{(opt)} + \varepsilon P_e^{(opt)}), \varepsilon > 0$. In addition, this conclusion also holds without the "optimal" condition. That is, for any decomposition determined by Eq. (14), conclusion (a) is valid.

For conclusion (b), let

$$\rho_x = \rho_b^{(opt)} + \frac{1 - S}{S}(P_e^{(opt)} - P_e'), \tag{15}$$

or equivalently,

$$S\rho_x + (1 - S)P_e' = S\rho_b^{(opt)} + (1 - S)P_e^{(opt)}. \tag{16}$$

The right-handed of Eq. (16) is just the optimal decomposition of ρ. We already know that S is the largest η of all possible decomposition (cf Eq.(14)). If the mixture on the left-hand of Eq.(16) does represent ρ, the weight of ρ_x must be less than S. In other words, the

left-hand of Eq.(16) can not be a real L-S decomposition about ρ. Hence $\rho_x \notin \mathcal{S}$. Theore, either ρ_x can not be positive, or can represent a non-separable state. The conclusion (b) can be demonstrated in Fig. 2. Of course the "optimal" condition is necessary in this case.

So far we have discussed the boundary of the set of all separable states. Using this concept, we give straightforward explanations for some entanglement measure of the mixed states, mainly for L-S decomposition. We feel that introducing boundary may be helpful for better understanding of entanglement.

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Figure Caption

Fig. 1 P_e (point A) denotes an entangled pure state. ρ (point B) represents a given non-separable mixed state. $\mathcal{S}$ is the set of all separable states. ρ_s (point C) is in the interior of $\mathcal{S}$ and ρ_b (point D) is on the boundary of $\mathcal{S}$.

Fig. 2 $P_e^{(opt)}$ and P_e' are two different entangled pure states. $P_e^{(opt)}$ and $\rho_b^{(opt)}$ construct the optimal L-S decomposition of ρ. ρ_x is outside of set $\mathcal{S}$. P_e' and ρ_x does not construct the L-S decomposition of ρ.
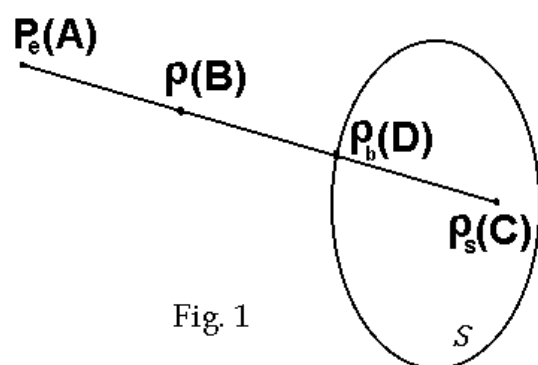
P$_e$(A)

ρ(B)

ρ$_b$(D)

ρ$_s$(C)

Fig. 1

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